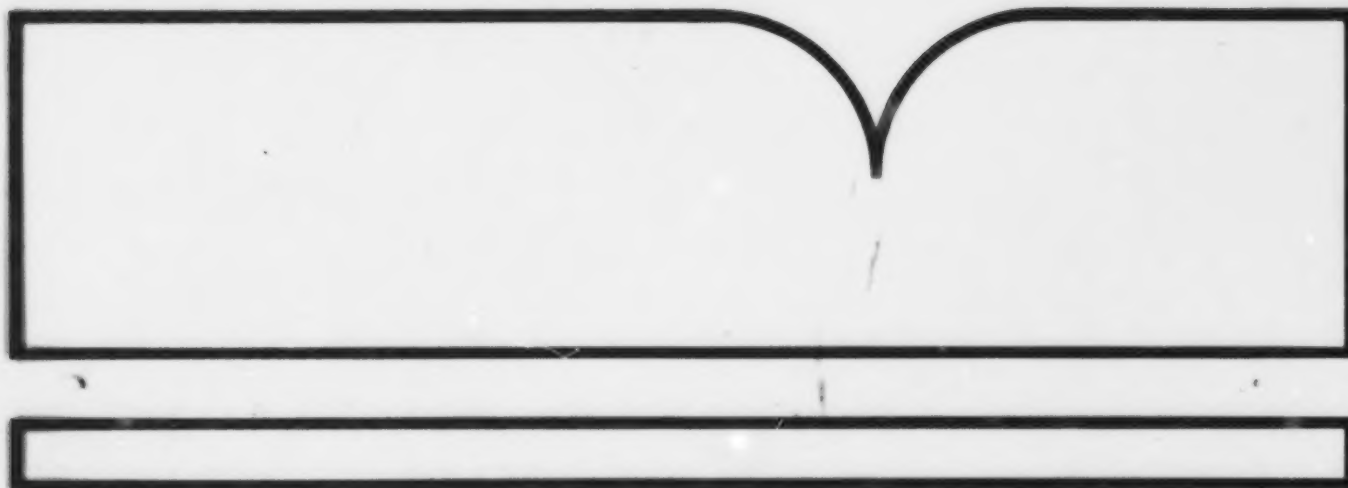


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Dynamic Estuary Model Performance

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DYNAMIC ESTUARY MODEL PERFORMANCE

By Robert B. Ambrose, Jr.¹ and Stephen E. Roesch²

ABSTRACT: Applications of the Dynamic Estuary Model (DEM) to both the Delaware and Potomac Estuaries by the Environmental Protection Agency during the 1970s are summarized and evaluated. Methods for calibrating, refining, and validating this model, and statistics for evaluating its performance are discussed. Following a brief description of DEM, observed and predicted hydrodynamic, mass transport, and water quality variables are statistically analyzed for the Delaware and Potomac applications. Weaknesses in the model and in these applications are identified. Model performance is evaluated for its usefulness to investigations of wastewater management alternatives in tidal rivers and the upper reaches of estuaries. Results indicate that the DEM can describe real-time longitudinal tidal hydraulics with good accuracy for relatively steady flow periods and can predict longitudinal mass circulation with sufficient accuracy for well-mixed, far-field conditions. The DEM can adequately predict relative differences in water quality to be expected from incremental wastewater management alternatives, but more realistic kinetic structures are needed to predict water quality response to large changes in waste load characteristics.

INTRODUCTION

Water quality models are now crucial elements of many applied water quality studies and planning programs. Case study evaluations, however, are needed to help engineers and managers choose appropriate models for their particular application.

The Central Regional Laboratory (CRL), of EPA's Region III, applied the Dynamic Estuary Model (DEM) to the Delaware and Potomac Estuaries and, in multiyear studies, refined the model to fit large and expanding data bases (1-5,13). The DEM is representative of the large class of "link-node" estuary models whose principal advantages (flexibility of application) and disadvantages (numerical dispersion) are generally known (9). This report evaluates how well the DEM simulates historical hydrodynamic, mass transport, and water quality data in the Delaware and Potomac Estuaries. We hope to inform future users of the capabilities and limitations of both this moderately complex model and the intermediate level of technology it represents.

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Rivers and Their Problems

The Delaware and Potomac Estuaries are drowned river valleys, typical of the MidAtlantic states. Well-defined heads-of-tide are located at the fall line between the piedmont and coastal plain. Semidiurnal tides dominate the primarily longitudinal ebb and flood currents. Freshwater inflow, averaging 3,000–4,000 m³/sec at the fall lines, controls the net seaward advection. Wind stress adds a significant stochastic variation. Depths are naturally shallow, and dredging is required to maintain navigational channels. The major metropolitan centers of Philadelphia, Pa. and Washington, D.C. are located along the fresh, tidal

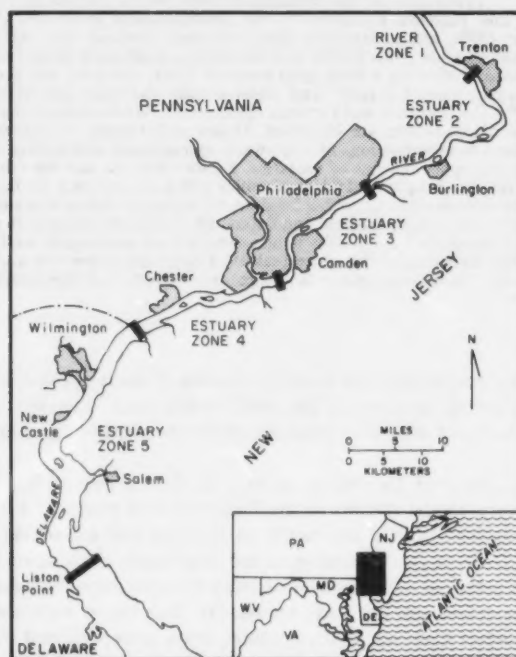


FIG. 1.—Delaware Estuary

river reaches of the Delaware and Potomac, respectively, and significantly affect their water quality.

The Delaware Estuary is operationally defined as the 140 km stretch between the fall line at Trenton, N.J., and the upper Delaware Bay at Liston Point, Del. (Fig. 1). Despite the primary wastewater treatment facilities installed by Philadelphia in the 1950s, thousands of tons of municipal and industrial wastewater from the Philadelphia-Camden-Chester complex still degraded the water dramatically throughout the 1960s and 1970s. Recovery begins as the tidal river widens into a broad, brackish estuary near Wilmington. A healthy balance is generally

restored as the estuary merges into Delaware Bay some one to three months travel below the fall line at Trenton.

The Potomac Estuary is operationally defined as the 182 km stretch between the fall line at Chain Bridge (in Washington) and Piney Point (Fig. 2). The large volume of sewage from the Washington metropolitan area has degraded the tidal river since the early 1800s. Treatment facilities constructed in the

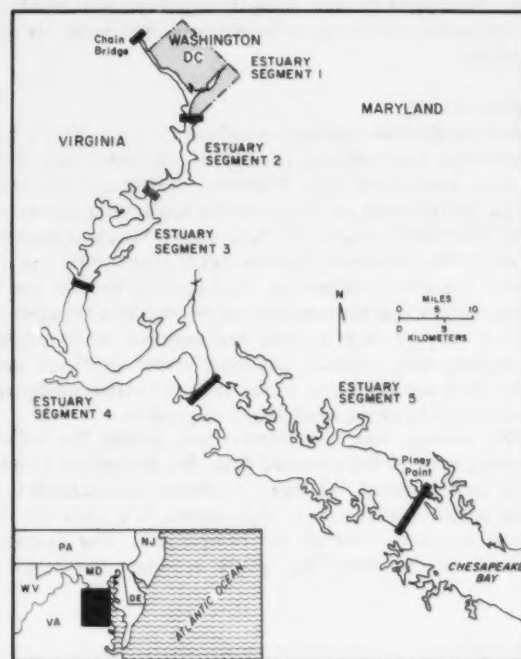


FIG. 2.—Potomac Estuary

1930s and upgraded in the 1970s have alleviated the most severe problems. A healthy balance slowly is being restored to most segments of the river.

Modeling Goals

The objective of CRL's applied hydrodynamic and mass transport studies has been to describe the real-time longitudinal circulation patterns of the tidal, freshwater, and upper estuarine reaches of the particular water bodies being examined. The resulting information is needed to drive water quality models for investigating wastewater management strategies. The hydrodynamic and mass transport models, then, had to reproduce the range of expected flow conditions, but not predict changing circulation patterns resulting from altered system geometry.

The objective of CRL's applied water quality studies has been improved understanding of the important water quality interactions in the particular water bodies being examined. The writers followed an iterative strategy of model use in which data are compared to model output, giving a set of errors that guide refinement of the model until the errors become acceptably small (7). The goal was a specific knowledge of how the particular water body behaves and the simplest possible model that describes this behavior. The resulting model was to provide a framework for examining the significance of trends in historical data and for forecasting future trends based on a reasonable set of cause and effect relationships.

Model Evaluation Strategy

To complement qualitative engineering judgment of how well a water quality model was calibrated and verified, the use of objective statistical measures is becoming more widespread (15). Statistical evaluations can serve both as a diagnostic tool for the engineer during model application and as an objective statement of model credibility for the decision-maker. Standard point comparisons alone can be misleading, however, because small phase shifts can lead to large calculated errors. Statistical analyses in the frequency domain can bypass this problem; finding relevant comparisons that can be interpreted in a process oriented context, however, may be more helpful. For example, when simulating a dye release, the engineer may compare observed versus predicted movement of the dye peak to check net advection, or the observed versus predicted spreading of the dye cloud width to check longitudinal dispersion.

Our evaluation strategy was to determine how closely the DEM simulated statistical characteristics of the observed data. We did not try to infer whether the model could be considered "validated," because that concept is useful only in reference to specific management applications. We used the same set of simple statistical parameters for all our comparisons. The average error, $\bar{E}$, and its associated relative error, RE, gauge accuracy and reveal systematic errors:

$$\bar{E} = \frac{1}{N} \sum_{i=1}^N (P_i - O_i) \quad \dots \quad (1)$$

$$RE = \frac{\bar{E}}{\bar{O}} \quad \dots \quad (2)$$

in which O_i = observed data; P_i = predicted data; $\bar{O}$ = observed data mean; and N = number of data points. The standard error of estimate, SE, and its coefficient of variation, CV, measure the precision with which the model tracks data variations:

$$SE = \left[\frac{1}{N} \sum_{i=1}^N (P_i - O_i)^2 \right]^{1/2} \quad \dots \quad (3)$$

$$CV = \frac{SE}{\bar{O}} \quad \dots \quad (4)$$

We then calculated linear regression statistics:

$$O_i = a P_i + b \dots \dots \dots (5)$$

The slope, a , measures the accuracy with which the model follows observed trends. The intercept, b , can point out systematic errors in the model. The correlation coefficient, r , measures the precision with which the model reproduces trends.

Dynamic Estuary Model

The DEM, developed by Water Resource Engineers, provides the capability for "real-time" simulations of the hydrodynamic and water quality behavior of an estuary (8). It has two components. The first is a hydrodynamic model that describes the tidally varying flows, velocities, and volumes throughout the estuary. The second is a quality model that describes the transfer, decay, and biochemical transformation of constituents in the estuary. Both components are referenced to a "link-node" network, representing the geometrical configuration of the estuary in a flexible, numerically simple manner.

The hydrodynamic model solves equations describing the propagation of a long wave through a shallow water system. It assumes that the flow is predominantly one-dimensional and that acceleration normal to the direction of flow, channel bottom slopes, coriolis forces, longitudinal density gradients, and wind forces are all negligible. Although the one-dimensional forms of the momentum and continuity equations are used, the link-node networks allow simplified representation of complex, branching estuarine geometry, with some limited lateral resolution.

The water quality model uses the data generated by the hydrodynamic model and performs a mass balance that includes kinetic decay and transformation processes for each parameter. The governing equation is expressed in a mass flux form, allowing evaluation between any pair of nodes. This gain in flexibility is countered, however, by a loss of stability due to the hyperbolic form of the equation, which tends to propagate errors. Stability is maintained through dissipation in the numerical solution procedure, an explicit, finite difference Euler technique. This dissipation, or "numerical dispersion," causes inaccuracies in the solution that can be only partially controlled.

Hydrodynamics

We calibrated the hydrodynamic model to each estuary using yearly average data to remove the significant short-term influence of wind stress, which is not included in this model. After imposing the yearly average tidal wave at the seaward boundaries of the models, and the yearly average tributary flows at the upstream boundaries, we spatially varied Manning's " n " to obtain good agreement for the ranges of water elevation and the timing of high and low water throughout the estuaries. Good, complete data on cross-sectional average tidal velocities and flows, however, are difficult to obtain. Consequently, maximum ebb and flood velocity data were checked against model calculations, but not used to recalibrate the model. Predicted maximum velocities represent averages over a channel cross-section and 1 to 2 km length, and thus should be smaller and less variable than reported maximum velocities, which are measured at a point.

We compared the predicted tidal responses with observed yearly average

values as a function of distance along the Delaware and Potomac Estuaries (16,17). For the Potomac comparisons, we pooled three additional data sets representing: (1) The yearly average spring tide; (2) January, 1971; and (3) June, 1971. Errors and regression statistics for the tidal ranges, high and low water arrivals, lengths of ebb tidal flow, and maximum tidal velocities are listed in Table 1.

The writers judged these hydrodynamic descriptions to be of sufficient quality to proceed with the mass transport and water quality phases of these studies.

TABLE 1.—Hydrodynamic Model Results for Delaware and Potomac Estuaries

Tidal response variable (1)	Calculated Errors					Regression Statistics		
	N (2)	$\bar{E}$ (3)	RE (4)	SE (5)	CV (6)	a (7)	b (8)	r (9)
(a) Delaware Estuary								
Tidal range, in meters	15	-0.012	-0.00	0.093	0.02	1.03	-0.06	0.98
High water arrival, in minutes	15	-18.4	-0.09	19.9	0.10	0.94	-6.69	1.00
Low water arrival, in minutes	15	-1.27	-0.01	7.6	0.03	0.99	0.32	1.00
Ebb flow, in minutes	12	-8.3	-0.02	22.9	0.05	0.42	25	0.94
Maximum flood velocity, in meters per second	12	-0.20	-0.21	0.28	0.29	0.56	0.22	0.69
Maximum ebb velocity, in meters per second	12	-0.37	-0.34	0.40	0.37	0.85	-0.21	0.70
(b) Potomac Estuary								
Tidal range, in meters	82	-0.001	-0.00	0.036	0.06	0.92	0.046	0.98
High water arrival, in minutes	82	0.076	0.02	0.27	0.07	0.97	0.03	0.99
Low water arrival, in minutes	82	0.025	0.01	0.22	0.05	0.98	0.07	1.00
Maximum flood velocity, in meters per second	15	-0.01	-0.04	0.16	0.23	0.37	0.44	0.54
Maximum ebb velocity, in meters per second	15	0.03	0.10	0.15	0.23	0.40	0.37	0.67

An important limitation to be kept in mind, however, is the model's restriction of the hydrodynamics to a constantly recurring, "stationary-state" solution (some versions of the DEM do handle transient hydraulics). This eliminates explicit consideration of short-term stochastic transients such as wind stress or large storm flushing, and complicates analysis of longer term patterns such as the two-week spring-neap-tide cycle or the seasonal freshwater inflow pattern. The model, then, is most reliable when predicting high and low values for diurnal, or tidal cycles, or both, averaged over a relatively steady two-week period. Despite this limitation, "real-time" simulations of water quality are possible,

but a scatter of data about the predictions is expected. This scatter is quantified in the mass transport phases of these studies.

Mass Transport and Circulation

The two most important processes affecting the circulation of dissolved conservative matter in well-mixed estuaries are net advection and longitudinal dispersion. Advection transports matter with the same velocity as the water; net advection is the average of this movement over a whole number of tidal cycles. Longitudinal dispersion includes not only small scale mixing phenomena such as eddy diffusion, but also complicated larger scale advection phenomena such as shear flow dispersion arising from lateral and vertical velocity gradients and density currents. Other advection phenomena arising from correlations between tidal oscillations in velocity, salinity, and cross-sectional area are sometimes lumped as "tidal dispersion." These separate processes, called "tidal pumping" and "tidal trapping," are calculated explicitly by real-time branching models and are not included in their dispersion coefficients (9).

Calibration and testing of the transport model required slack-water data describing the intertidal movement of salinity (or chloride ion) and dye tracer. Salinity data were chosen from historical steady flow periods of various magnitudes and durations. Dye data were gathered in the estuaries following short, controlled point releases. The salinity data describe net upstream mixing within the lower, brackish reaches, whereas the dye data describe instantaneous downstream mixing subject to transient flow through the upper, freshwater reaches. Calibration, testing, and verification of the transport model proceeded using "real-time" simulations of these historical time periods.

After imposing observed chloride concentrations at the boundaries of the models, we varied an advective and a dispersive parameter, FACTOR and C_d , to reproduce observed concentration profiles. The predicted chloride profiles were compared with observed data during several steady flow periods in the Delaware and Potomac Estuaries. Errors and regression statistics are listed in Table 2. These statistics should be interpreted with caution because of the relatively few data points and the influence of the lower boundary on the calculated concentrations.

The real time dye tracer simulations are perhaps more rigorous tests of the model's advective and dispersive transport mechanisms. We compared predicted dye profiles with observed data at several slack tides following discharge of the tracer into freshwater reaches of the Delaware and Potomac Estuaries. Because we made no adjustments to the advection and dispersion parameters, these simulations constitute a further verification of the models' transport components. Pooling all the data sets for each estuary, the writers calculated errors and regression statistics for the net downstream movement of the dye peak, the buildup and attenuation of the peak dye concentration, and the spreading of the $0.1 \mu\text{g/L}$ dye isocline.

To inspect the Delaware model's advection and mass dilution performance more closely, we divided the dye simulation into two periods. The first eight days were influenced by low freshwater flows; during this period the dye discharge becomes well mixed in the river. The second 13 days were influenced by higher, transient freshwater flows, and the well-mixed dye cloud was advected downstream. The coefficients of variation for the peak concentration and location

TABLE 2.—Transport Model Results for Delaware and Potomac Estuaries

Transport response variable (1)	Calculated Errors					Regression Statistics		
	<i>N</i> (2)	$\bar{E}$ (3)	RE (4)	SE (5)	CV (6)	<i>a</i> (7)	<i>b</i> (8)	<i>r</i> (9)
(a) Delaware Estuary								
Chloride concentration, in milligrams per liter	35	-140.	-0.10	440.	0.31	0.97	-98.	0.97
Movement of 500 milligrams per liter isochlor, in kilometers	5	-1.9	-0.22	2.8	0.33	0.78	-0.05	0.99
Peak dye concentration, in $\mu\text{g/L}$								
All data	14	0.03	0.09	0.10	0.30	0.82	0.09	0.82
Period 1	7	0.06	0.14	0.14	0.32	0.52	0.27	0.62
Period 2	7	0.01	0.05	0.03	0.14	0.76	0.07	0.92
Movement of dye peak, in kilometers								
All data	14	3.4	0.26	6.0	0.45	1.12	1.8	0.96
Period 1	7	1.6	0.54	5.1	1.73	0.15	4.2	0.44
Period 2	7	5.0	0.21	6.6	0.28	1.26	-1.1	0.98
Width of 0.1 $\mu\text{g/L}$ dye isocline, in kilometers								
All data	14	1.3	0.05	3.2	0.13	0.83	5.5	0.90
Period 1	7	1.0	0.04	2.3	0.10	0.84	4.5	0.96
Period 2	7	1.6	0.06	4.0	0.14	0.38	20.0	0.47
(b) Potomac Estuary								
Chloride concentration, in milligrams per liter	37	-85.	-0.02	200.	0.05	0.95	300.	1.00
Dye concentration, in $\mu\text{g/L}$								
All data	189	0.00	0.00	0.12	0.44	0.69	0.08	0.84
Period 1	50	0.11	0.27	0.18	0.44	0.68	0.05	0.81
Period 2	139	-0.03	-0.14	0.08	0.37	0.85	0.06	0.85
Peak dye concentration, in $\mu\text{g/L}$	14	-0.01	-0.01	0.15	0.22	0.96	0.02	0.91
Movement of dye peak, in kilometers	14	-0.9	-0.14	1.4	0.22	0.98	1.0	0.97
Width of 0.1 $\mu\text{g/L}$ dye isocline, in kilometers	10	1.9	0.10	1.3	0.07	0.66	4.5	0.96

were significantly lower during the second period than the first (14% and 28% versus 32% and 173%, respectively). Real time simulations of near-field spiked concentrations, then, cannot predict observed data with high precision. Real time simulations of far-field, damped concentration peaks, however, can predict observed data with good precision, even under transient hydrodynamic conditions.

These simulations demonstrate how the models were able to handle the important transport processes of net advection, mass dilution, and longitudinal dispersion. We judged the transport descriptions to be of sufficient quality to proceed with the water quality phases of these studies. Certain limitations, however, should be kept in mind. It would be difficult to calibrate water quality constituents with much greater precision than demonstrated by the transport components. The precision of the transport components is limited by the models' hydrodynamic descriptions, considered earlier, and by the lack of lateral resolution. Consequently, predictions of observed data following transient discharges will be imprecise until lateral mixing is complete. This mixing process depends on the location within the estuary, but requires approximately a week.

Water Quality

The final goal of most applied modeling studies is to predict changes in water quality resulting from changes in management strategies under an expected range of natural conditions. The water quality problem of most concern in the Delaware Estuary has been the low dissolved oxygen (DO) concentrations during the summer and early fall. A major purpose of this Delaware study was to provide a sounder basis for relating proposed waste load allocation schemes to estuarine DO concentrations. The water quality problems of most concern in the Potomac Estuary have been the high algal blooms associated with excessive enrichment and the moderately low DO concentrations during hot weather periods. A major purpose of this Potomac study was to clarify the relationship between Blue Plains' discharge of nutrients and the estuary's maximum algal levels.

The data collection programs associated with these studies included intensive, synoptic surveys, long-term trend surveys, and special field and laboratory studies (3,4,5). The intensive, synoptic surveys—here composed of "slack-water" sampling runs, station transect sampling, and diurnal sampling—formed the backbone of our data collection efforts. Although rather expensive to conduct, these two-week to one-month surveys can yield a good, complete data base for extracting cause-effect relationships (10,12).

Special field and laboratory studies can measure many important kinetic rates. We were cautious in applying this type of data to represent actual, in-situ processes because of the many possible modifying factors not present nor accounted for in the special studies. We used these rate studies to help establish permissible ranges through which we could vary the kinetic rates during the calibration process. Of course, the more precise and accurate the rate measurement, the more the calibration range was constrained.

Delaware Calibration and Test Results.—Our initial model, based largely on the Delaware Estuary Comprehensive Study (DECS) (6), is shown in Fig. 3. The writers studied five independent data sets in the process of calibration and testing: July, 1974; October, 1973; August, 1975; summer, 1968; and July, 1976. The data cover a significant range of both waste loading conditions and summer/fall flow and temperature conditions (3). We used the first three sets

of data to calibrate the water quality model. The fourth data set comprised of three periods in summer, 1968, and the fifth data set collected in July, 1976, were used strictly for model verification. The sequential model formulations that were pursued during the course of this study are summarized in Table 3. The final model formulation is shown in Fig. 4.

A statistical comparison of observed and predicted median concentrations by river zone is presented in Table 4. The most important variable, DO, displayed a minor -0.15 mg/L absolute error and a standard error of 0.68 mg/L. The coefficient of variation of 0.18 can be compared with values of 0.31 and 0.14 for chloride concentrations and well-mixed peak dye concentrations predicted by the transport model. As expected, the verification performance deteriorated from calibration, with standard errors about 50% higher. Predictions of the DO minimum were unbiased; the average error is less than 0.1 mg/L, but the standard error exceeds 0.5 mg/L. The model predicts the length of estuary suffering concentrations below 2 mg/L and 4 mg/L with standard errors of 6 and 9 km, respectively, out of a total 140 km.

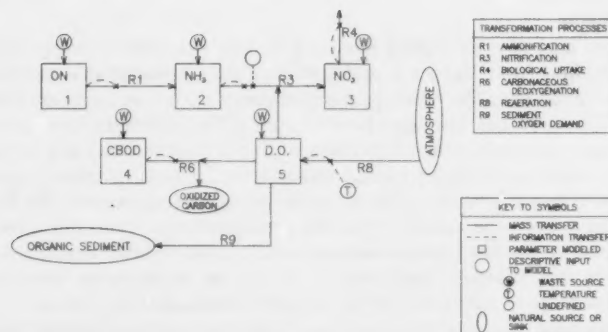


FIG. 3.—Initial DEM Kinetic Structure for Delaware Estuary

Accurate BOD data are perhaps the most difficult to obtain. Although the model predicts carbonaceous BOD, available 30-day uninhibited BOD data reflect nitrification and algal respiration. We found neither a correlation between BOD_5 and BOD_{30} nor a satisfactory way to separate the BOD_{30} into separate components. Consequently, we compared BOD_{30} data with UBOD calculated by the following formula:

$$UBOD = CBOD + 4.3 \times (ON + NH_3) + 0.02 \times CHL \dots \dots \dots (6)$$

in which CHL = phytoplankton chlorophyll a in $\mu\text{g/L}$, and all other concentrations are in mg/L . The ratio, $0.02 \text{ mg DO}/\mu\text{g CHL}$, assumes that half of algal carbon is degraded in the BOD test and that the phytoplankton average about $0.03 \text{ mg C}/\mu\text{g CHL}$. Despite the lack of local data to support these assumptions, the average underprediction of BOD was only 0.7 mg/L , and the standard error and coefficient of variation were only 1 mg/L and 0.15 , respectively. The 0.93 correlation coefficient indicates that the model was able to explain 86% of the observed zonal variability.

TABLE 3.—Overview of Delaware Model Calibration Phase

Step (1)	Model performance problems (2)	Processes added to model structure or functions (3)
1	Poor NH_3 match (July, '74)	Chemical inhibition of nitrification around Philadelphia
2	NO_3 overpredicted (July, '74)	Biological uptake, NO_3 to ON
3	Total N overpredicted (July, '74)	Settling of ON near large discharges. Denitrification when $\text{DO} < 1$
4	Poor NH_3 match (Oct., '73)	Lengthened zone of nitrification inhibition as function of lower temperature
5	DO "sag" too deep, not prolonged, or flat (July, '74)	Reduced SOD when $\text{DO} < 2$. Link denitrifying NO_3 as oxygen source for CBOD decomposition
6	Calibrated rates differ (July, '74 and Oct., '73)	Add temperature correction factors; use same set of rates, corrected to 20°C
7	DO drastically underpredicted (Aug., '75)	Link observed chlorophyll <i>a</i> bloom to DO through calibrated <i>P</i> and <i>R</i> rates, observed euphotic depth, temperature, and photoperiod; add algal rates to July, '74, Oct., '73
8	DO slightly overpredicted (July, '74, Oct., '73)	Readjust CBOD deoxygenation and settling rates slightly, maintaining Aug., '75 algal rates applied to observed July, '74 and Oct., '73 chlorophyll <i>a</i> and euphotic depth

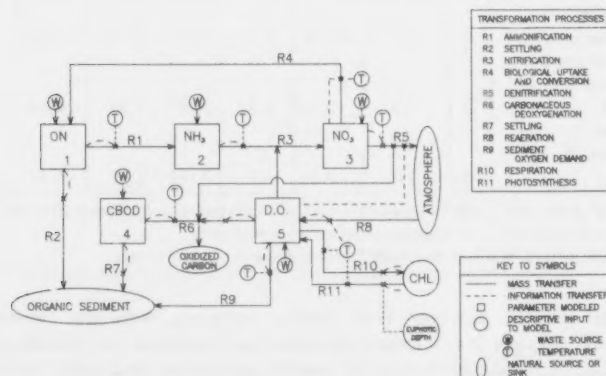


FIG. 4.—Final DEM Kinetic Structure for Delaware Estuary

Despite the difficulties in simulating the nitrogen cycle with variable nitrification inhibition, predicted concentrations compared satisfactorily with observed data. Standard errors between 0.16 mg/L and 0.24 mg/L correspond to CVs between 0.17 and 0.37. The pronounced ammonia (NH_3) and nitrite plus nitrate (NO_3) gradients were reproduced, for the most part, by the model. The small variations

TABLE 4.—Water Quality Model Results for Delaware Estuary

Quality response variable (1)	Calculated Errors					Regression Statistics		
	N (2)	$\bar{E}$ (3)	RE (4)	SE (5)	CV (6)	a (7)	b (8)	r (9)
(a) Median Concentrations, in milligrams per liter ^a								
DO	36	-0.15	-0.04	0.69	0.18	0.84	0.44	0.93
UBOD	8	-0.70	-0.11	0.97	0.15	0.84	0.37	0.93
NH_3	36	0.05	-0.10	0.16	0.33	0.90	0.10	0.91
NO_3	36	-0.11	-0.08	0.24	0.17	0.90	0.04	0.91
ON	36	-0.11	-0.19	0.21	0.37	0.14	0.39	0.27
(b) DO Categories								
Zone 2, in milligrams per liter	9	-0.21	-0.04	0.50	0.10	0.78	0.90	0.91
Zone 3, in milligrams per liter	9	0.13	0.06	0.66	0.28	1.21	-0.38	0.78
Zone 4, in milligrams per liter	9	-0.10	-0.04	0.82	0.32	0.82	0.35	0.86
Zone 5, in milligrams per liter	9	-0.41	-0.08	0.73	0.15	0.74	0.87	0.92
Calibration, in milligrams per liter	16	-0.06	-0.02	0.53	0.14	0.88	0.39	0.95
Verification, in milligrams per liter	20	-0.22	-0.06	0.79	0.21	0.81	0.47	0.92
DO Minimum ^b , in milligrams per liter	9	-0.07	-0.05	0.55	0.41	1.54	-0.79	0.78
2 milligrams per liter reach length, in kilometers ^c	9	-2.7	-0.13	6.0	0.28	0.90	-0.64	0.89
4 milligrams per liter reach length, in kilometers ^c	9	2.1	0.04	9.3	0.16	1.04	-0.16	0.86

^aConcentrations are medians by river zone (>30 km) and survey period (9 total).

^bMedian concentration at minimum station or model node.

^cRiver kilometers in which DO falls below indicated concentration.

in the flat organic nitrogen (ON) profile, however, were not reproduced. Fortunately, changes in ON have little impact on predicted DO concentrations.

Sensitivity analyses exploring the model parameters and rates found DO concentrations to be most sensitive to algal parameters—euphotic depth, photosynthesis (P) and respiration (R) rates, and chlorophyll *a* concentrations—and to the regeneration rate, but not to the deoxygenation rate (3). Analyses confirmed

that, whereas carbonaceous deoxygenation presently is the most important oxygen sink overall, nitrification is of equal importance in uninhibited reaches above and below Philadelphia (1). Sediment oxygen demand (SOD) is significant throughout the estuary, but more so immediately below the fall line at Trenton and around the major discharges at Philadelphia. Although water quality in the freshwater reaches between Trenton and Philadelphia is dominated by upstream conditions during high flow periods, roughly half of the oxygen deficit during low flow periods can be attributed to local wastewater discharges. The large municipal wastewater loads at Philadelphia cause most of the oxygen depletion in the critical reaches at and below Philadelphia during moderate and low flow periods. Effects can be felt as far downstream as Delaware.

Certain nonlinear model features were necessary to match model calculations with observed data taken between 1968 and 1976. Large reductions in CBOD wastewater loadings were achieved during this time span, but water quality improvements were disappointing. The writers' interpretation was that low DO affects the SOD and denitrification rates, requiring larger reductions in wastewater to bring the DO concentrations from 1 mg/L to 2 mg/L than from 3 mg/L to 4 mg/L. Management options must take into account the implied higher costs of cleanup.

Potomac Calibration and Test Results.—As a starting point for our Potomac water quality study, we used the results of the CRL surveillance and modeling program conducted between 1965 and 1975 (2). This program provided the basis for the DO standards promulgated for the Potomac Estuary. More recently, the Potomac has been studied by investigators from Hydrosience (14) and The Massachusetts Institute of Technology (11). These past studies have elucidated several water quality processes important to the Potomac Estuary's nutrient, algal, and DO budgets: the dominant role of nitrogen as the historical limiting nutrient, the importance of nitrification to DO levels and in influencing the location of algal blooms, the importance of phytoplankton in driving both average DO levels and daily fluctuations, and the importance of turbidity in controlling the effects of phytoplankton on DO. Remaining questions concerning the potential roles of phosphorus, carbon, and light penetration in limiting phytoplankton under current and future management schemes, the role of sediments in the nitrogen and phosphorus budgets, and the relative importance of domestic sewage loads versus stormwater runoff during both dry and wet weather periods are under study by CRL, the Washington Council of Governments, and the United States Geological Survey.

The writers decided to first evaluate how well the early Potomac DEM (Fig. 5) simulated the available data from 1965 to 1975, then to recalibrate the model to scrutinize how well the old structure could incorporate the new, more intensive data bases of 1977 and 1978 (4,5). Two main factors were expected to cause a deterioration in model performance between the early and the late data sets. First is the change in the Potomac itself. The model structure was formulated with data from the early period, when Blue Plains was a conventional secondary treatment plant. Evidence pointing to nitrogen limitation was reflected in the model. In early 1977, however, phosphorus removal was put on line at Blue Plains in an attempt to lower estuary phosphorus levels to a level that would limit phytoplankton growth. Any large changes in the nutrient balance probably would not be simulated accurately by the early model.

The second factor causing deterioration in model performance is the nature and use of the data sets. The early data were averaged over steady periods, then compared with stationary (dynamic steady-state) model output for the constant flow and temperature conditions. The later data intensively described a given time period and were compared with real time model output for the varying flow and temperature conditions. In comparing the model with the later data, then, the writers were evaluating its ability to describe some of the dynamics of eutrophication.

A statistical comparison of observed and predicted median concentrations by river segment for the early data is presented in Table 5. REs ranged from -1%-11%, CVs from 5%-46%, regression slopes from 0.75-1.11, and correlation coefficients from 0.70-0.99. Of special note was the exceptional job of predicting the chlorophyll peak, with an absolute error of $-4 \mu\text{g/L}$, a standard error of $6 \mu\text{g/L}$, a regression slope of 1.02, and a correlation coefficient of 0.99.

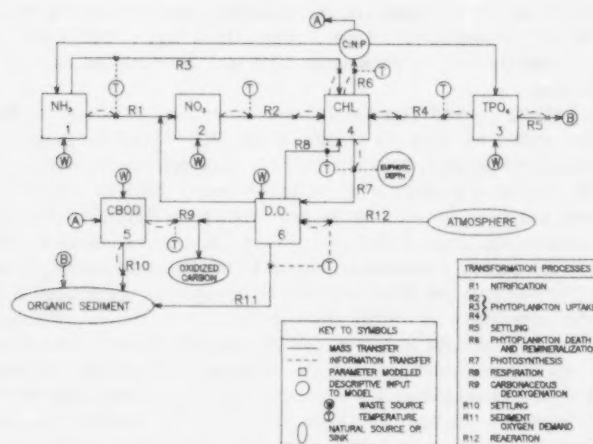


FIG. 5.—DEM Kinetic Structure for Potomac Estuary

After applying the model to the new data, it was immediately obvious that the simple phosphate component was totally inadequate in describing the new Potomac phosphorus regime. The phosphate system, then, was unlinked, and model evaluation proceeded for the nitrogen-phytoplankton-dissolved oxygen structure.

Without the phosphate component, predictions of chlorophyll *a* deteriorated, as shown by the statistical comparisons in Table 6. Chlorophyll *a* concentrations are spatially quite variable. This causes the high standard error of $53 \mu\text{g/L}$ (CV of 69%). Statistical comparisons between observed and predicted peak concentrations and locations, however, revealed better essential agreement. The peak concentrations were simulated with a $35 \mu\text{g/L}$ (23%) standard error, and an $11 \mu\text{g/L}$ (7%) systematic error. Predicted peak locations averaged 4.8 km upstream of observed peaks, with a standard deviation of 17.7 km. This high

TABLE 5.—Water Quality Model Results for Potomac Estuary, 1965–1975 Data

Quality response variable (1)	Calculated errors					Regression statistics		
	N (2)	$\bar{E}$ (3)	RE (4)	SE (5)	CV (6)	a (7)	b (8)	r (9)
(a) Median Concentration ^a								
DO, in milligrams per liter	32	-0.04	-0.01	1.02	0.17	0.80	1.12	0.86
NH ₃ , in milligrams per liter	41	0.02	0.02	0.27	0.31	1.01	0.01	0.95
NO ₃ , in milligrams per liter	39	0.05	0.07	0.18	0.26	0.79	0.21	0.90
TPO ₄ , in milligrams per liter (as PO ₄)	40	0.01	0.01	0.20	0.16	1.03	-0.03	0.98
CHL, $\mu\text{g/L}$	31	2.7	0.04	19.3	0.27	0.92	8.7	0.87
(b) Extreme Concentration ^b								
DO minimum, in milligrams per liter	9	-0.02	-0.01	0.35	0.23	1.08	-0.15	0.93
NH ₃ maximum, in milligrams per liter	15	-0.02	-0.01	0.20	0.11	0.91	0.15	0.96
NO ₃ maximum, in milligrams per liter	12	-0.11	-0.09	0.25	0.20	0.85	0.08	0.93
TPO ₄ maximum, in milligrams per liter (as PO ₄)	14	-0.15	-0.05	0.30	0.10	1.00	-0.16	0.97
CHL maximum, $\mu\text{g/L}$	8	-4.1	0.03	6.1	0.05	1.02	-7.1	0.99
(c) Reach Length ^c								
DO < 5 milligrams per liter	9	-2.1	-0.10	4.3	0.20	0.81	2.1	0.78
DO < 3 milligrams per liter	9	-1.1	-0.11	3.2	0.33	0.66	2.2	0.70
NH ₃ > 1 milli- grams per liter	15	1.7	0.08	6.8	0.32	0.93	3.2	0.94
NO ₃ > 1 milli- grams per liter	12	-0.3	-0.02	6.6	0.46	0.91	1.0	0.95
TPO ₄ > 1 milli- grams per liter (as PO ₄)	14	0.0	0.0	8.6	0.23	0.80	7.6	0.79
CHL > 100 $\mu\text{g/L}$	8	2.2	0.10	5.3	0.25	1.11	-4.5	0.95

^aConcentrations are median values by river segment (16–26 km) and survey period.^bMedian concentration during survey at minimum or maximum location.^cRiver kilometers in which concentration exceeds or falls below indicated value.

variability is a result of biological, rather than transport, processes. Concluding that the phytoplankton system needed updating, we made chlorophyll *a* a controlled exogenous variable and evaluated the remaining nitrogen-dissolved oxygen structure. Statistical results are given in Table 7.

Looking first at DO, we see that most of the performance statistics remain similar to those calculated for the old data. Although the DO minimum is predicted with the same overall accuracy in the new data, the four-fold increase in the SE shows a deterioration in the model's precision (or survey-to-survey consistency). This may be caused by a change in the character of the DO sag itself. The depression is less sharp and well-defined for the new data, with a minimum averaging 3.4 mg/L versus 1.5 for the old data. The length of estuary experiencing depressed concentrations was predicted at least as well for the new data as for the old. The high 166% CV for reach lengths below 3 mg/L is attributable

TABLE 6.—Chlorophyll *a* Model Results for Potomac Estuary, 1977–1978 Data

Quality response variable (1)	Calculated errors					Regression statistics		
	N (2)	$\bar{E}$ (3)	RE (4)	SE (5)	CV (6)	<i>a</i> (7)	<i>b</i> (8)	<i>r</i> (9)
Median concentration, ^a in $\mu\text{g/L}$	32	12.2	0.16	53.2	0.69	0.82	26.2	0.69
Peak concentration, in $\mu\text{g/L}$	8	11.3	0.07	35.1	0.23	1.16	-14.2	0.94
Peak location, ^b in ki- lometers	8	-4.8	-0.15	17.7	0.55	0.14	22.9	0.09
100 $\mu\text{g/L}$ reach length, in kilome- ters ^c	8	2.8	0.11	10.9	0.42	0.86	6.5	0.89

^aConcentrations are median values by river segment (16–26 kilometers) and survey period.

^bDistance of peak concentration below Blue Plains (river kilometer 16).

^cRiver kilometers in which concentration exceeds 100 $\mu\text{g/L}$.

to the low average observed length and is not indicative of how well the model predicted the DO sag.

As average ammonia concentrations declined three-fold from the old data to the new, the model's ability to predict median segment values remains roughly the same. The SE of 0.26 mg/L, with a CV of 107%, is somewhat misleading; the steep slopes of the observed and predicted profiles combined with slight phase shifts can dramatically influence these statistics. The peak concentration, by contrast, is predicted with an SE of 0.14 mg/L, with a CV of 13%. The predicted peak location averaged just 1.4 km upstream of the observed location; the SE of 7 km (267%), however, indicates natural variability not captured by the model. Recalling that the SE for the peak dye location was 1.4 km (22%), the writers conclude that the variability in the ammonia peak location is the result of chemical or biological processes. The reach length experiencing concentrations above 1 mg/L, predicted with an SE of 1 km and a CV of

39%, is not as sensitive to this variability. It may be recalled that dye widths, which are affected primarily by dispersive processes, were characterized by an SE of 1 km and a CV of 7%.

TABLE 7.—Water Quality Model Results for Potomac Estuary, 1977–1978 Data

Quality response variable (1)	Calculated Errors					Regression Statistics		
	N (2)	$\bar{E}$ (3)	RE (4)	SE (5)	CV (6)	a (7)	b (8)	r (9)
(a) Median Concentration, ^a in milligrams per liter								
DO	32	-0.20	-0.03	1.15	0.16	0.54	3.00	0.77
CBOD	29	-1.00	-0.31	1.57	0.48	0.25	1.47	0.33
NH ₃	29	-0.11	-0.45	0.26	1.07	0.38	0.04	0.59
NO ₃	40	-0.02	-0.03	0.15	0.24	0.85	0.08	0.97
(b) Extreme Concentration, ^b in milligrams per liter								
DO minimum	8	-0.03	-0.01	0.86	0.25	0.70	0.99	0.62
CBOD maximum	8	-0.26	-0.04	1.92	0.32	1.30	-2.09	0.66
NH ₃ maximum	10	0.04	0.04	0.14	0.13	0.89	0.15	0.95
NO ₃ maximum	10	-0.08	-0.05	0.18	0.11	0.90	0.10	0.85
(c) Extreme Location, ^c in kilometers								
DO minimum	8	-1.2	-0.10	3.7	0.31	1.02	-1.4	0.99
CBOD maximum	8	-6.0	-0.82	10.5	1.45	0.01	1.1	0.04
NH ₃ maximum	10	-1.4	-0.54	6.9	2.67	-0.03	1.2	-0.11
NO ₃ maximum	10	-2.4	-0.31	5.5	0.70	0.71	-0.2	0.89
(d) Reach Length, ^d in kilometers								
DO < 5 milligrams per liter	8	-3.2	-0.22	5.4	0.37	0.66	1.7	0.97
DO < 3 milligrams per liter	8	-0.4	-0.25	2.7	1.66	0.27	0.8	0.53
CBOD > 4 milligrams per liter	8	-12.7	-0.65	17.7	0.90	0.21	3.0	0.64
NH ₃ > 1 milligrams per liter	10	-0.2	-0.07	1.1	0.39	0.84	0.3	0.95
NH ₃ > 0.5 milligrams per liter	10	0.0	0.0	2.4	0.30	0.83	1.4	0.92
NO ₃ > 1 milligrams per liter	10	-2.7	-0.11	6.3	0.26	-0.03	21.9	-0.03

^aConcentrations are median values by river segment (16–26 km) and survey period.

^bMedian concentration during survey at minimum or maximum location.

^cDistance of extreme concentration below Blue Plains (river kilometer 16).

^dRiver kilometers in which concentration exceeds or falls below indicated value.

As nitrite plus nitrate concentrations have declined slightly, the model's ability to predict median segment concentrations, maximum concentrations, and the spatial extent of elevated concentrations has improved somewhat. Median concentrations were simulated with an SE of 0.15 mg/L and a CV of 24%.

The positive 0.08 mg/L regression intercept, combined with the slightly low 0.85 slope, show that not all of the observed variability in concentrations was captured by the model. The results are considered satisfactory.

ANALYSIS OF RESULTS

The Delaware Estuary application of the DEM yielded coefficients of variation between 2% and 10% for the most important hydrodynamic variables, between 13% and 45% for the important transport variables, and between 15% and 41% for the water quality variables. The Potomac Estuary application of the DEM gave coefficients of variation from 5%–7% for the hydrodynamics, 5%–44% for the transport, and 11%–267% for water quality. Excluding the tests overly biased by small phase shifts, the Potomac water quality response falls between 11%–90%. Errors in replicating observed conditions, then, increased some five-fold going from the hydrodynamic component of the model to the mass transport component. Errors in replicating observed conditions, not strongly affected by small phase shifts, increased two-fold or less going from the mass transport component of the model to the water quality component. When steep concentration gradients are produced by strongly coupled water quality variables, however, their interaction with the estuary's mass transport behavior produces a situation difficult to model with precision. Attempts to predict such concentrations at specific locations with the water quality component suffered errors up to six-fold higher than the mass transport component.

Correlation coefficients also showed the same trends. The Delaware application gave 94%–100%, 82%–99%, and 78%–93% for important hydrodynamic, transport, and water quality variables, respectively. The Potomac application yielded 98%–100%, 84%–100%, and –10%–99%. Again, excluding the same tests biased by phase shifts, the Potomac water quality response improves to between 33% and 99%.

In our judgment, these statistics reveal the DEM to be basically reliable when operated within the range of conditions for which it is calibrated and tested. The model is able to capture the overall trends nicely. Certain limitations, however, should be kept in mind. The model cannot reliably predict transient or steep concentration gradients with precision exceeding approximately five kilometers or three hours. Below these levels, the model is limited by its basic network and hydrodynamic properties. Above these levels, of course, the model is limited by the precision of the input data and the nature of the water quality structure implemented. In the Delaware application, for example, the model could not calculate the DO variations for a given day because hour-to-hour changes in phytoplankton concentrations and water clarity were not measured. Even if these important forcing functions had been measured with great precision, however, the model would still be limited by the inability of its present water quality structure to handle hour-to-hour changes in incident light, photosynthesis and respiration rates, and local wind-induced reaeration. So although the model will calculate hour-to-hour changes in water quality variables for every simulated day, results should be averaged to obtain average diurnal variability over a minimum of one or two week intervals within the simulated time period.

Problems also should be expected if the model is used to predict behavior significantly outside its test range. This includes large channel modifications,

water diversions, or radically different pollutant discharges. These situations should be analyzed with either special-purpose models or specialized adaptations to a general-purpose model like the DEM. Even then, extra care is required for extrapolating results beyond the model's test range.

An important example of the pitfalls of extrapolation is the troublesome, but not unanticipated, failure of the Potomac model to track the changing phosphorus regime given a 70% reduction in major phosphorus waste loads. The failure of the previously unimportant and thus simplified phosphorus component of the model resulted in deterioration of chlorophyll *a* and thus DO predictions as the upper estuary responded to the new nutrient balance. Efforts have been underway at CRL to update phosphorus kinetics to describe this new balance.

The writers consider the model to be capable of adequately predicting the relative differences in water quality to be expected from incremental wastewater management alternatives. This includes such options as consolidating individual wastewater treatment plants into a regional facility, relocating existing wastewater discharges, or incrementally reducing wastewater loads. Direct effects of nonpoint source load reductions can be evaluated. Indirect effects, such as changes in the sediment regime, can be handled with much less certainty. The ability to predict the response to large changes in waste load characteristics depends on improved kinetic components to the model.

The writers have most confidence when the model is used to explore the dominant interactions affecting current water quality conditions. These sensitivity analyses can provide valuable insight into the uncertainties associated with the management alternatives.

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APPENDIX II.—NOTATION

The following symbols are used in this paper:

- a = linear regression slope;
- BOD = biochemical oxygen demand;
- BOD₅ = five-day biochemical oxygen demand;
- BOD₃₀ = thirty-day biochemical oxygen demand;
- b = linear regression intercept;
- C = carbon concentration;
- C_d = dimensionless dispersion coefficient;
- CBOD = carbonaceous biochemical oxygen demand;
- CHL = phytoplankton chlorophyll a concentration;
- CV = coefficient of variation;
- DO = dissolved oxygen concentration;
- $\bar{E}$ = average error;
- FACTOR = dimensionless advection parameter;

- N = number of data points;
- n = Manning's channel roughness coefficient;
- NBOD = nitrogenous biochemical oxygen demand;
- NH_3 = ammonia nitrogen concentration;
- NO_3 = nitrite plus nitrate nitrogen concentration;
- $\bar{O}$ = mean of observed data;
- O_i = observed data point i ;
- ON = organic nitrogen concentration;
- P = algal photosynthesis rate;
- P_i = predicted data point i ;
- R = algal respiration rate;
- RE = relative error;
- r = correlation coefficient;
- SE = standard error of estimate;
- SOD = sediment (or benthic) oxygen demand rate;
- t = time;
- TPO_4 = total phosphorus concentration, as phosphate;
- UBOD = ultimate biochemical oxygen demand; and
- x = distance along longitudinal axis.